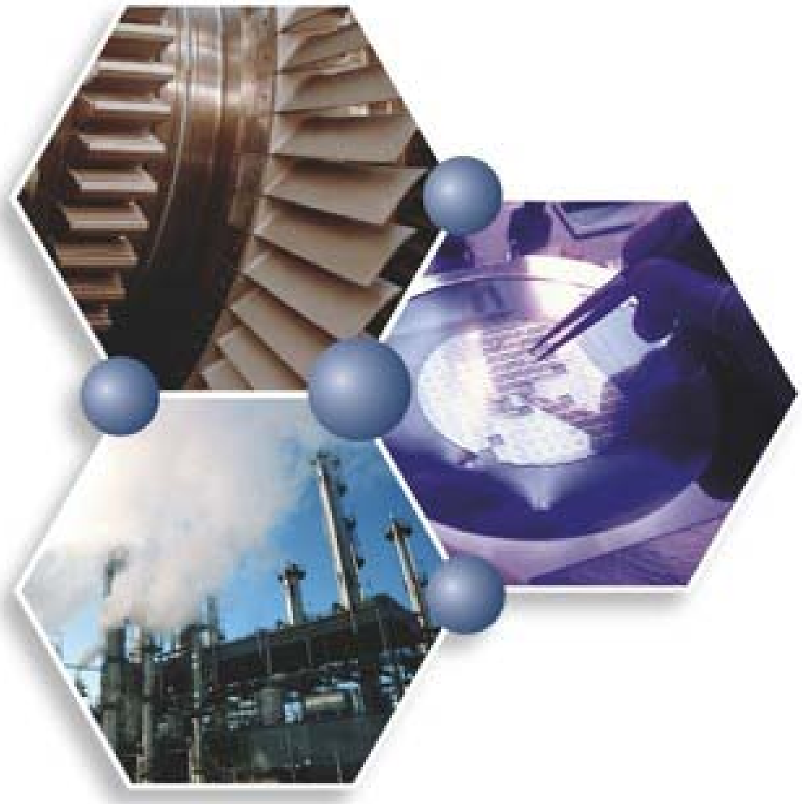


What's New with CHEMKIN

Ellen Meeks

4th Biennial International Workshop on CHEMKIN in Combustion

Chicago, IL

July 25, 2004

REACTION DESIGN

Outline

- What's New with CHEMKIN 4.0
  - New user interface
  - Reactor network diagrams
  - New and enhanced reactor models
- Introducing KINetics/API
- Model Fuels Consortium initiative
- Future of this Workshop

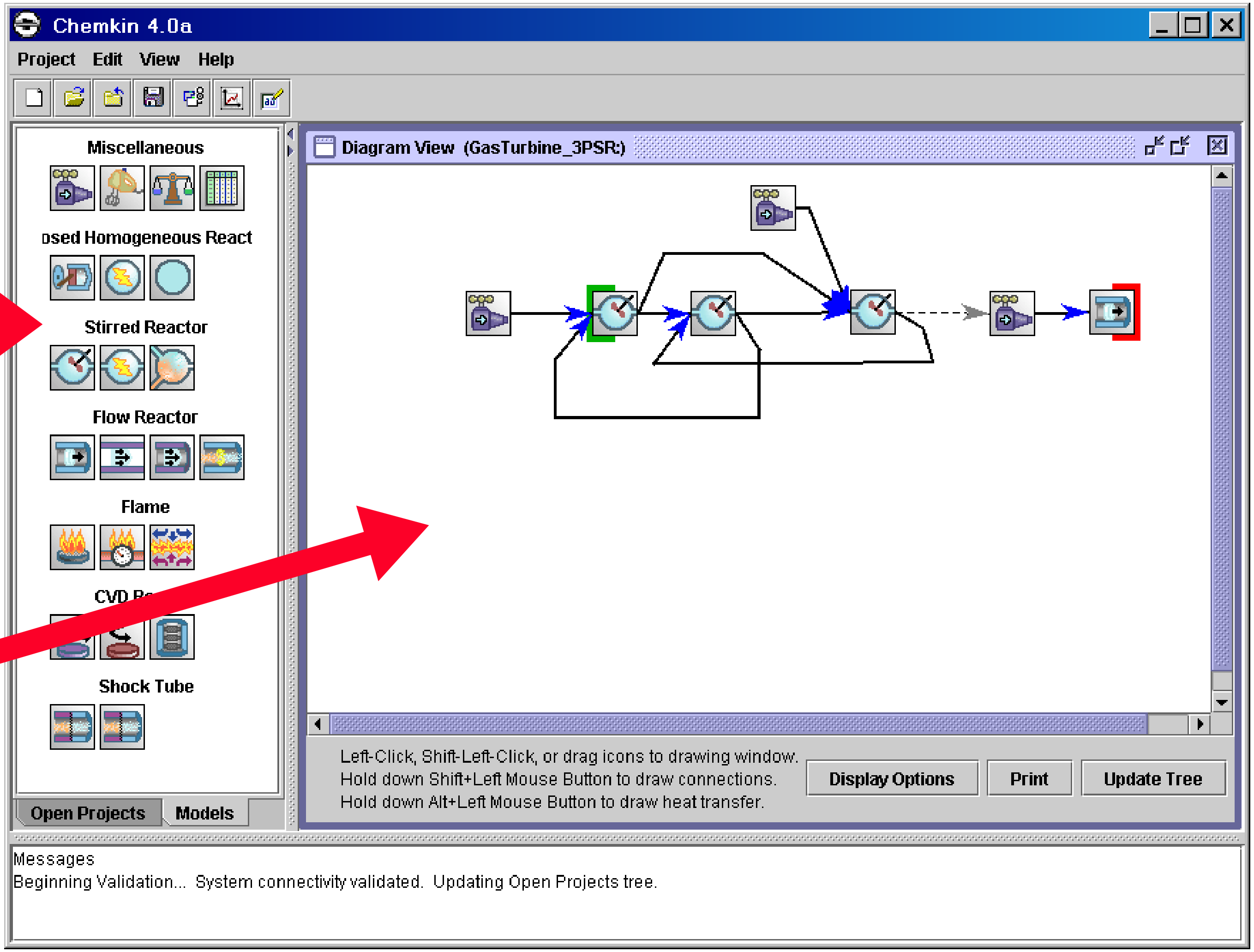
CHEMKIN 4.0 has arrived

- New Graphical User Interface
- Visual linking of modules to form reactor networks
- New transient simulation capability
- Expanded plug-flow capability
- Expanded partially stirred reactor capability
- New reaction-rate types
- And much more...

Users can build reactor networks through a visual interface with array of reactor models

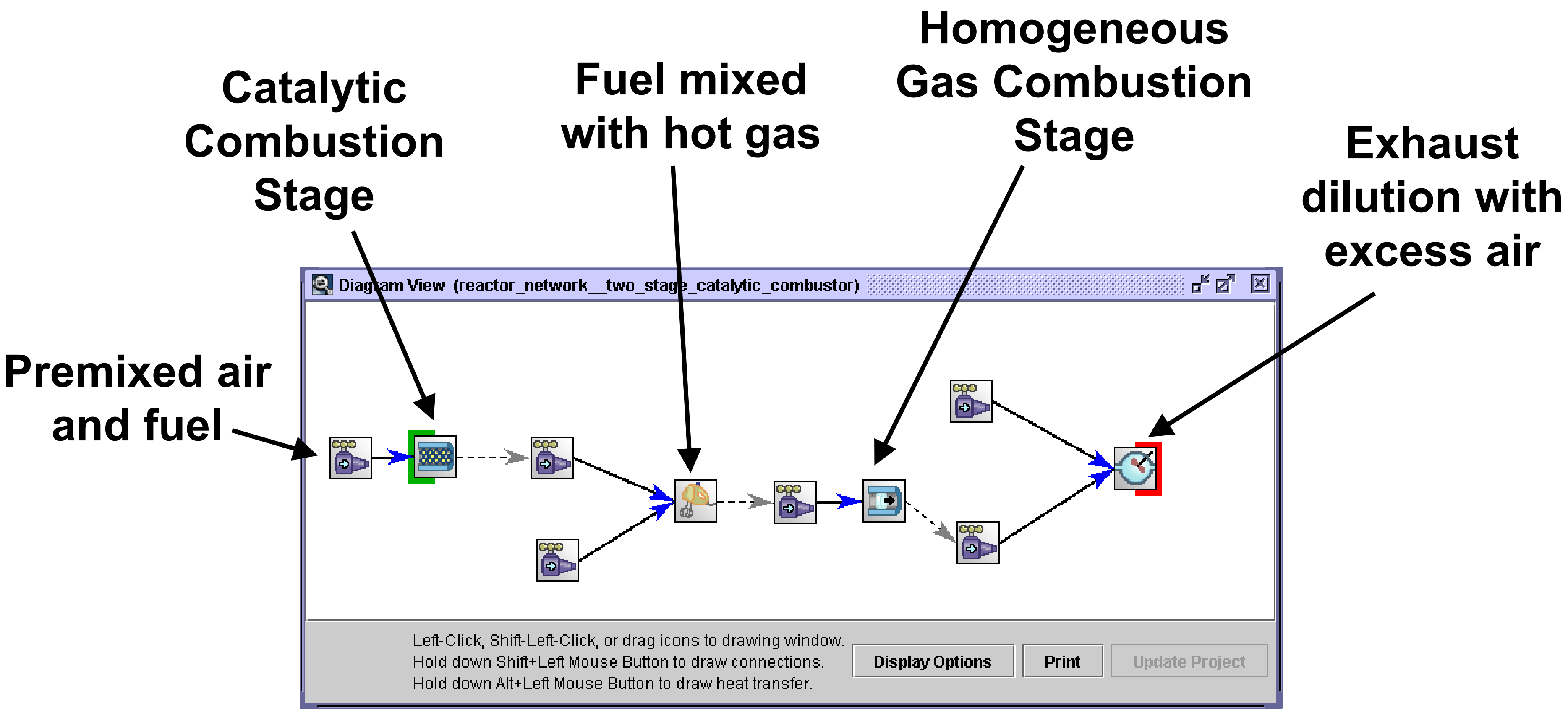
Customizable palette of reactor modules

Drag and drop diagramming tool for reactor networks and series simulations



Model of a two-stage combustor demonstrates one use of reactor networks

- Diagram for simulation easily built in User Interface

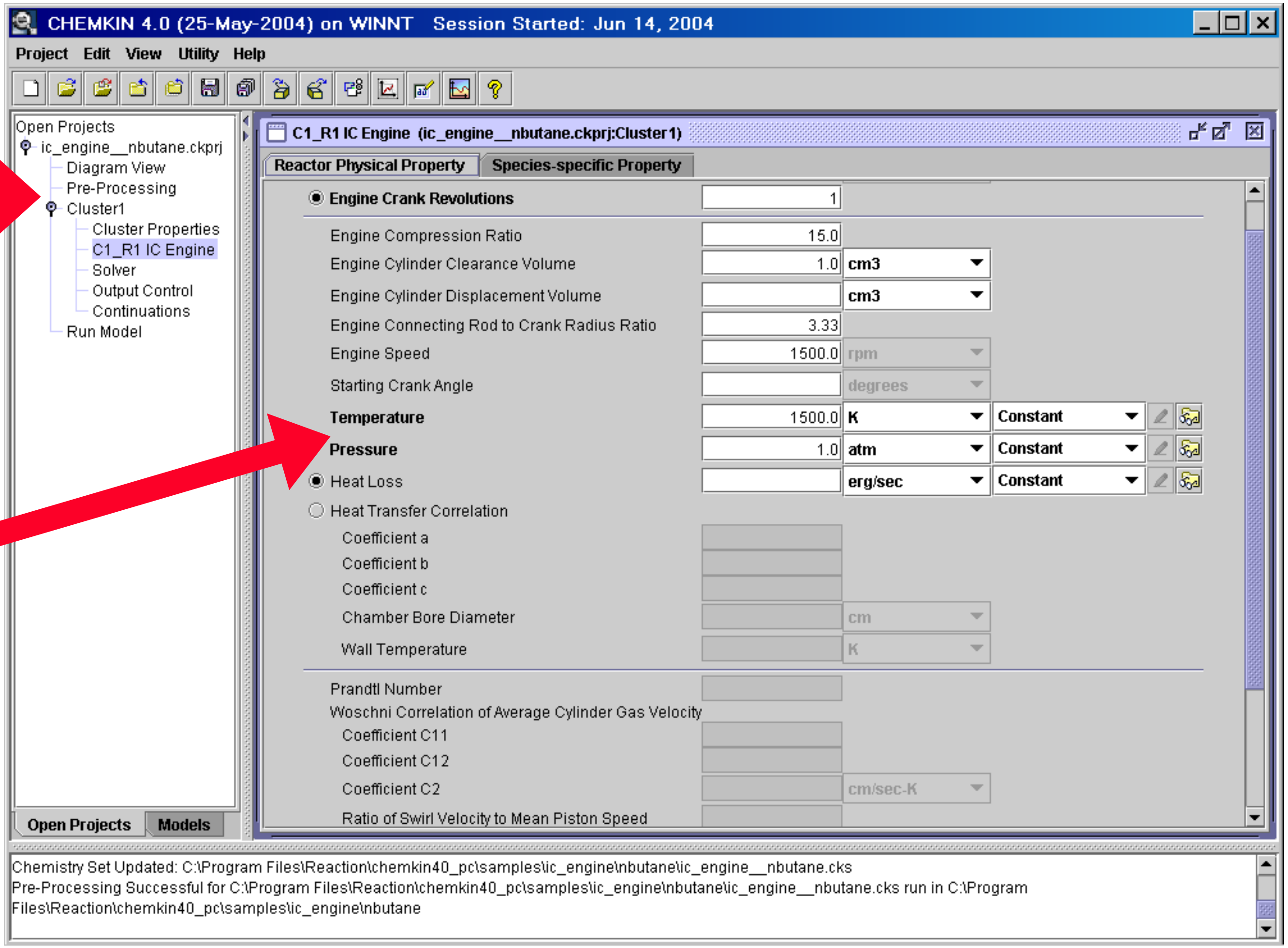


Descriptions of reactor configurations are through context-specific panels

- (No keywords required!)

Project tree with links to input panels

Input panels guide problem set-up and execution



REACTION DESIGN

Templates for Reactor Models guide user inputs for problem-specific applications

- Reactor Models include:

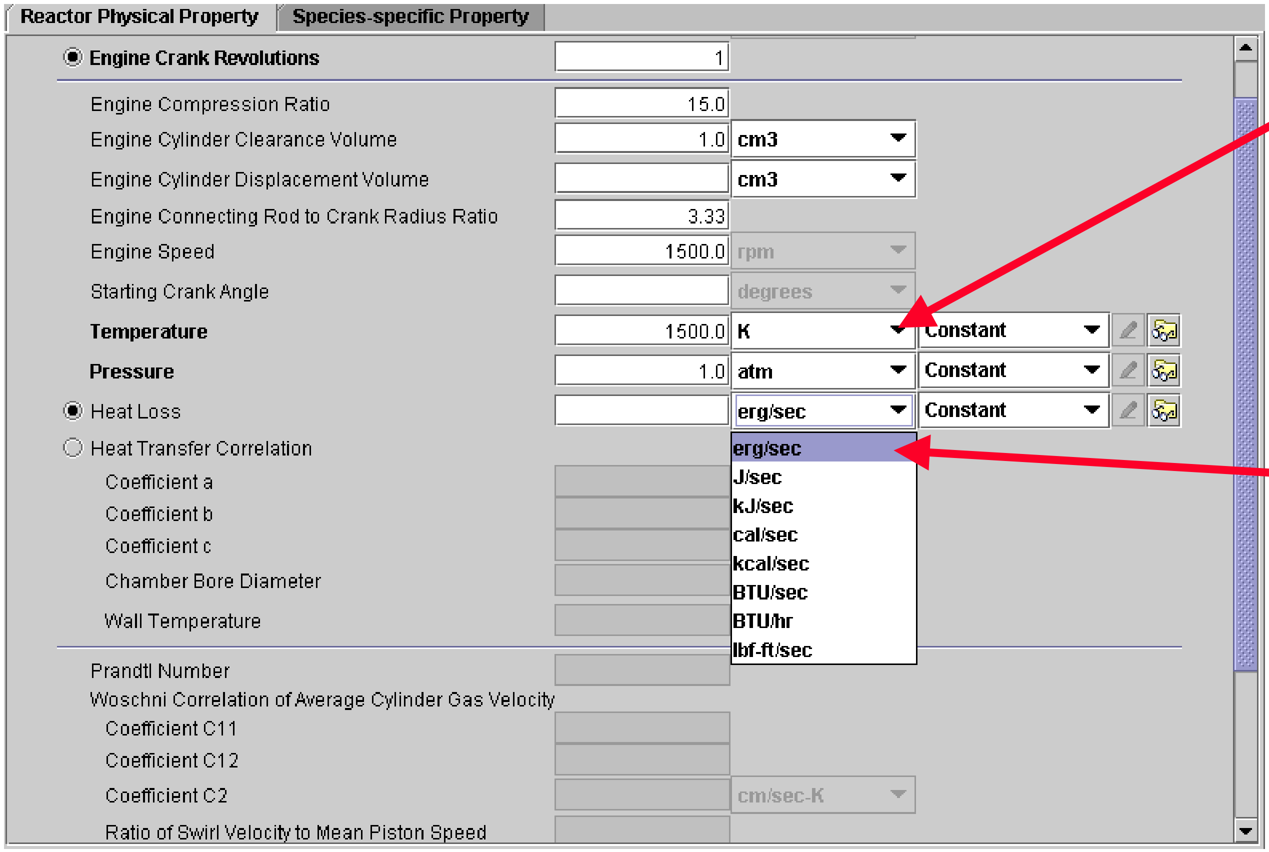
	Non-reactive Gas Mixer
	Chemical and Phase Equilibrium Calculations
	Mechanism Analyzer
	Closed Internal Combustion Engine Simulator
	Closed Homogeneous Batch Reactor
	Closed Partially Stirred Reactor
	Closed Plasma Reactor
	Perfectly Stirred Reactor (PSR)
	Plasma PSR
	Partially Stirred Reactor (PaSR)
	Plug Flow Reactor

	Honeycomb Plug Flow Reactor
	Plasma Plug Flow Reactor
	Planar Shear Flow Reactor
	Cylindrical Shear Flow Reactor
	Premixed Laminar Burner-stabilized Flame
	Premixed Laminar Flame-speed Calculation
	Diffusion or Premixed Opposed-flow Flame
	Stagnation Flow CVD Reactor
	Rotating Disk CVD Reactor
	Normal Incident Shock

Reaction Design

Users have a wide array of options in physical units for input parameters

- SI, cgs, British, and user-customized options



Pull-down menus provide context-specific options

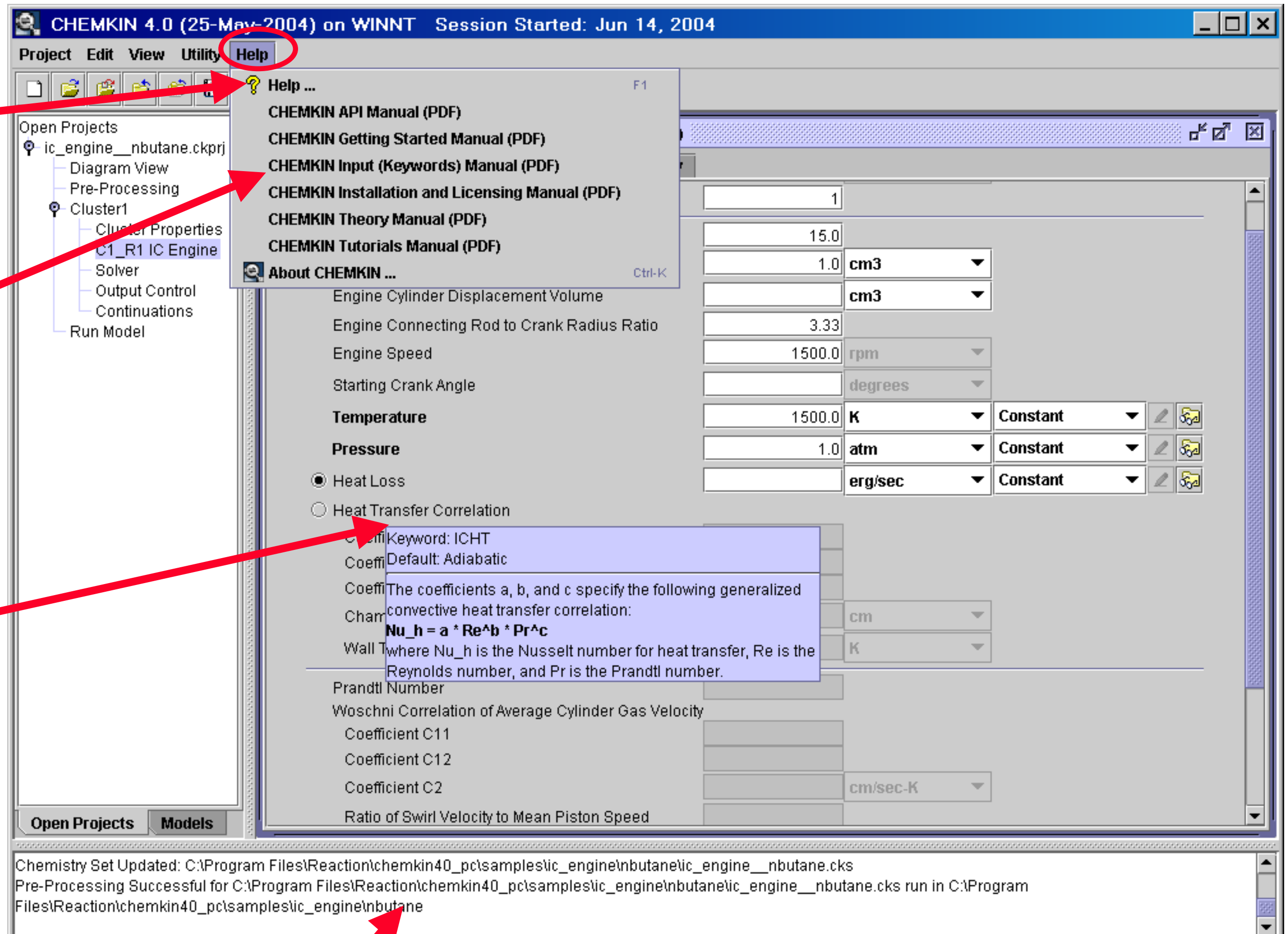
Defaults based on user preferences

Online Help includes context-sensitive bubble help, HTML, and PDFs

HTML Help for overview of GUI features

In-depth user manuals

Quick-reference, mouse-over “bubble” help



Diagnostic messages

User manuals have been reorganized to accelerate the CHEMKIN learning curve

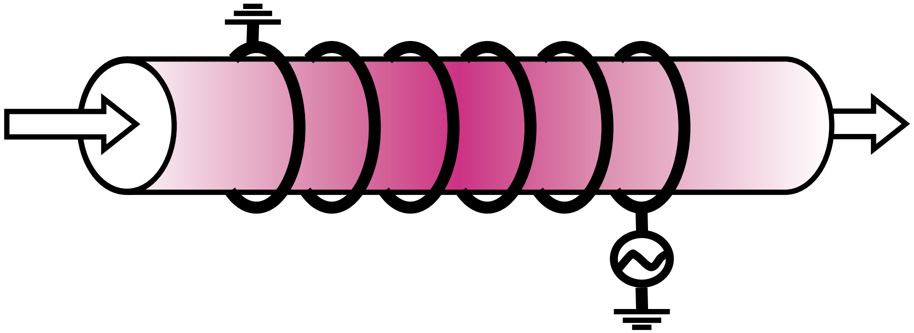
- Installation and Licensing
  - System Administrators guide to installation and license setup
- Getting Started using CHEMKIN
  - Overview of the new user interface, post-processing, and command-line scripting
- Program Input
  - Detailed description of all user input parameters, including reactor, kinetic, thermodynamic, and transport data
- Tutorials
  - Problem-oriented samples
- CHEMKIN/API
  - Programmer’s guide for linking external programs to CHEMKIN
- Theory
  - Underlying equations, assumptions, and references

CHEMKIN plug-flow capability has been greatly expanded

- Sensitivity analysis as function of distance
  - Species, temperature, and velocity
  - Gas-phase reaction rates
  - Surface reaction rates
- More robust solver
- More easily linked to other reactors
- Restart and continuation options
- Radiation exchange with external environment

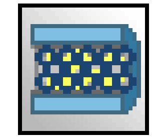
New plasma plug-flow reactor for plasma abatement and downstream-etch applications

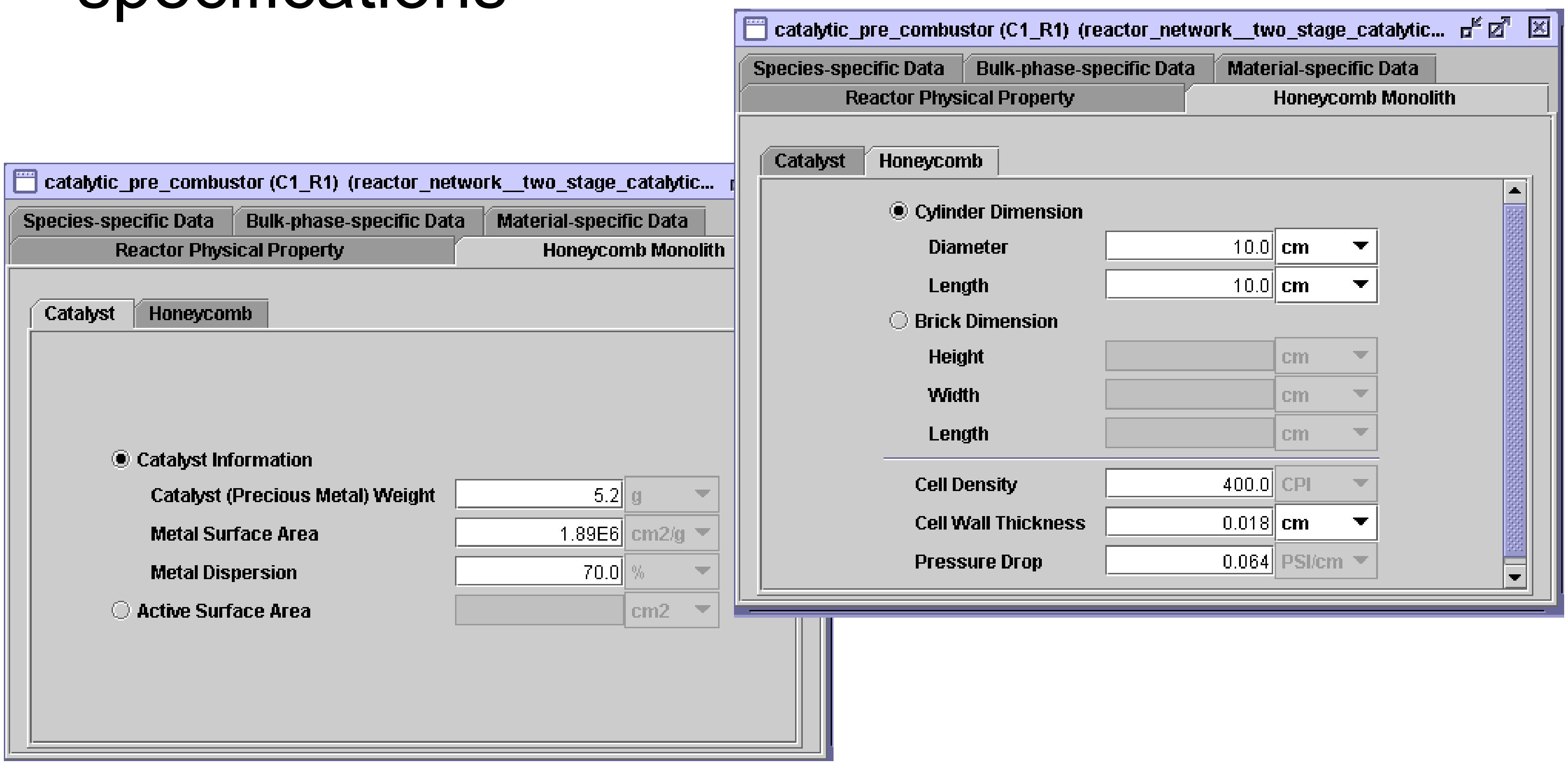
- Power can vary along length of channel
- Electron energy equation to determine mean electron temperature
  - Under plug-flow assumptions
- Electron and ion driven reactions
- General plasma-surface reaction capability



Honeycomb reactor model allows users to specify catalyst monolith properties

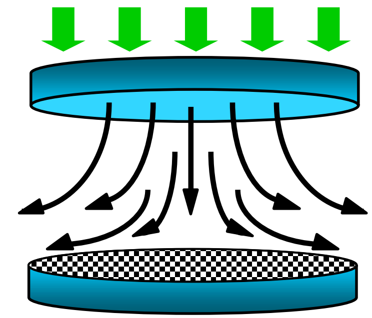
- Active surface area for catalytic reactions calculated automatically from catalyst specifications

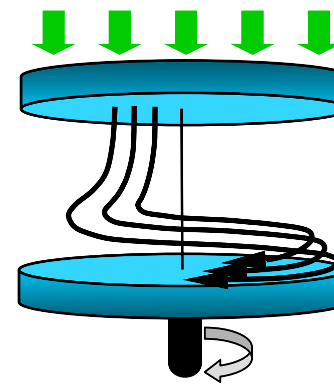




New transient stagnation-flow and rotating-disk reactor models

- Atomic layer deposition
- Multiple inlet streams
  - Different temperatures & compositions
  - Different velocities
- Inlet streams vary as function of time
  - Pulsed or cycled
  - User-specified flow-rate profiles
- Robust alternative to reach steady-state for difficult problems

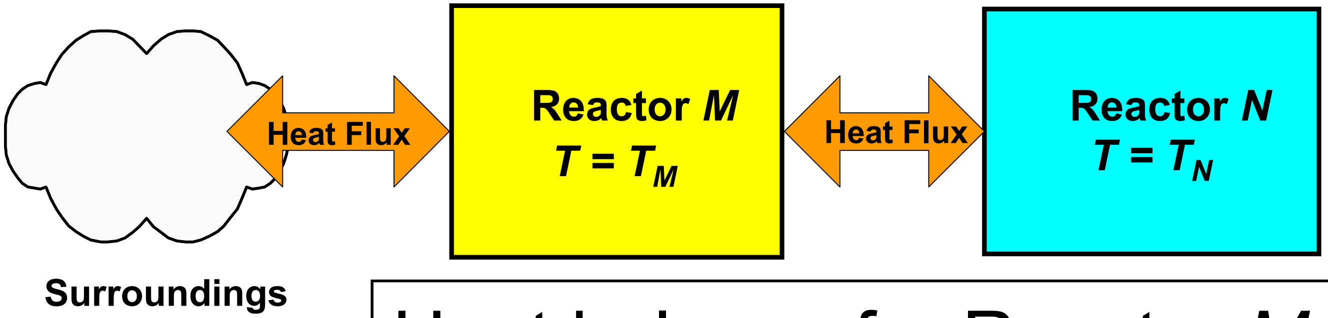




Reaction Design

Network of homogeneous reactors (PSRs) can now include heat transfer between zones

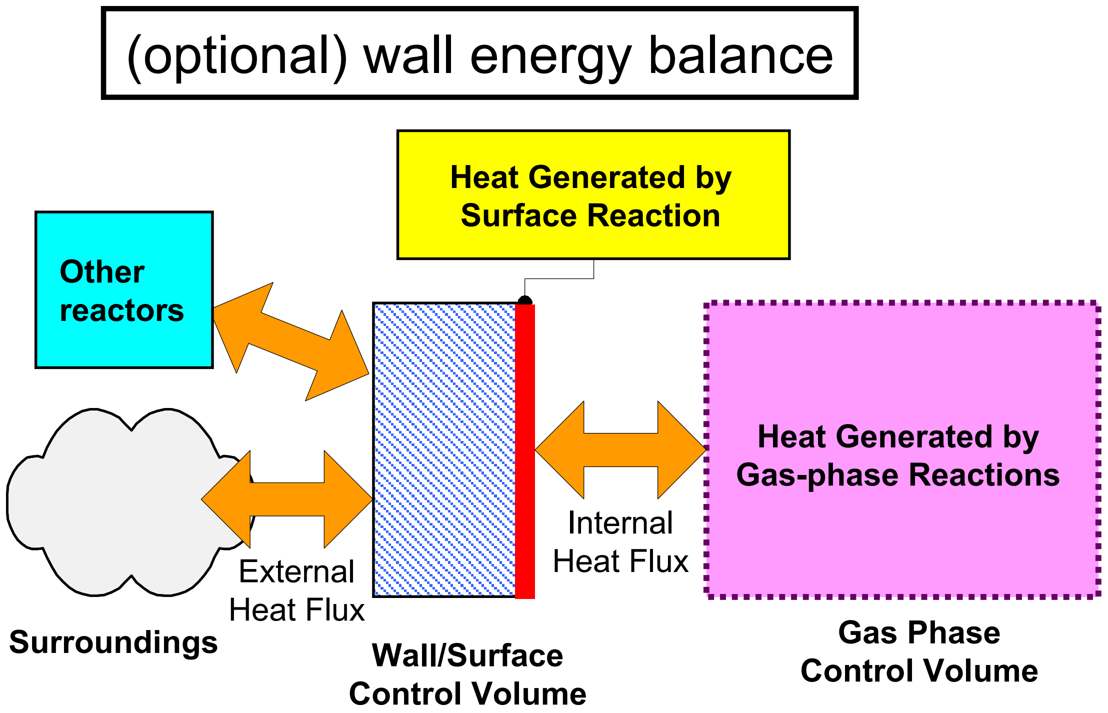
- General heat exchange capability
  - Radiation
  - Conduction or convection
  - From any reactor to any other reactor



Heat balance for Reactor *M*

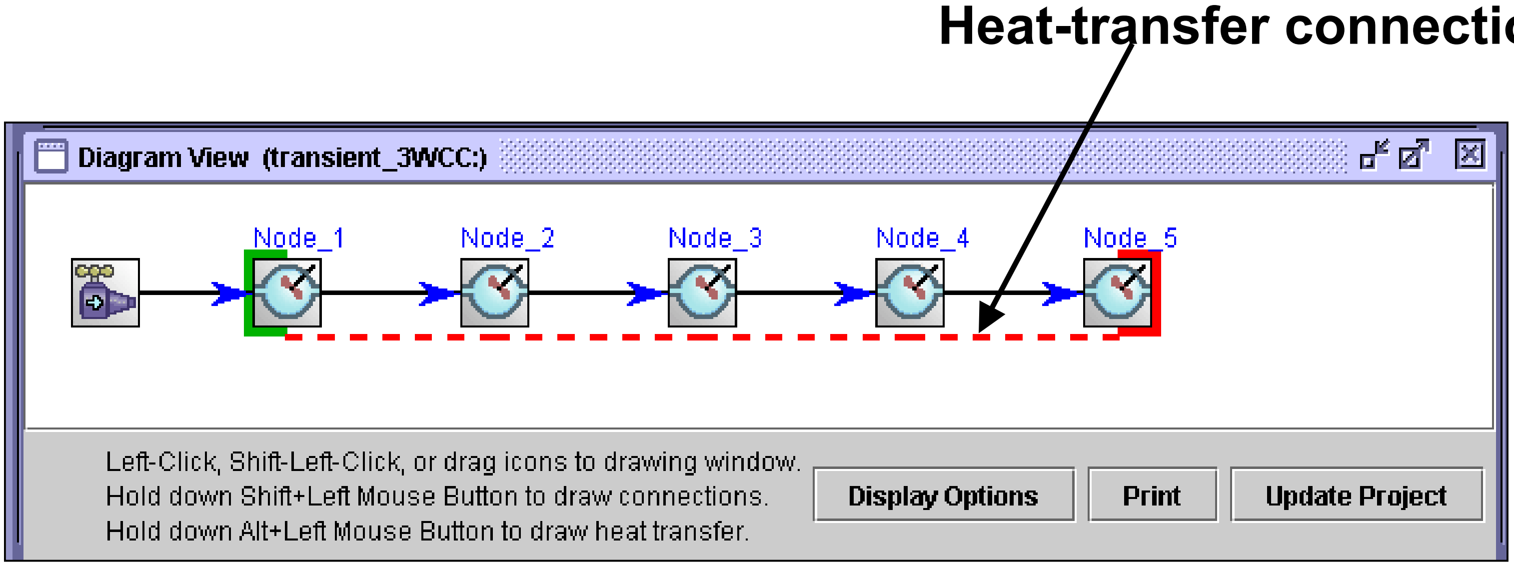
Transient (PSR) reactor networks can account for solid wall heat capacity

- Allows simulation of complex systems with heat and mass balance
- User specified heat-capacity for wall



Transient plug-flow can be modeled with a series of PSRs

- Heat capacity can be included
  - e.g., to reproduce lag of catalyst bed temperature
- Diffusion and conduction upstream can be modeled through heat-transfer coefficient between PSRs



The Partially Stirred Reactor capabilities have been expanded

- Reactor can be characterized by any combination of volume, flow rate, residence time
- Volume can be specified as a function of time
- Multiple inlet streams are allowed
- A PaSR reactor stream can be initialized by a previous PaSR solution
- Closed-system PaSR model
- Users can request output of probability-distribution functions and scatter-plot data for any number of variables

We have improved management of very large chemistry mechanisms

- User may filter sensitivity data prior to running
  - By species name
  - By relative “tolerance” value
  - Greatly reduced solution-file size and post-processing time
- GetSolution post-processing utility enhanced
  - Generates plain text files for import/export
  - User filtering options for data export
  - Access from Graphical User Interface
- Improvements to transient solver
  - Added solver method options
  - Optimized solution strategy for closed reactors
  - 10X+ speed-up in sensitivity analysis

New reaction rate formulations provide added flexibility in describing chemistry

- Langmuir-Hinshelwood & Eley-Rideal surface-reaction formulations:
  - Example:

    A + B $\Rightarrow$ C + D

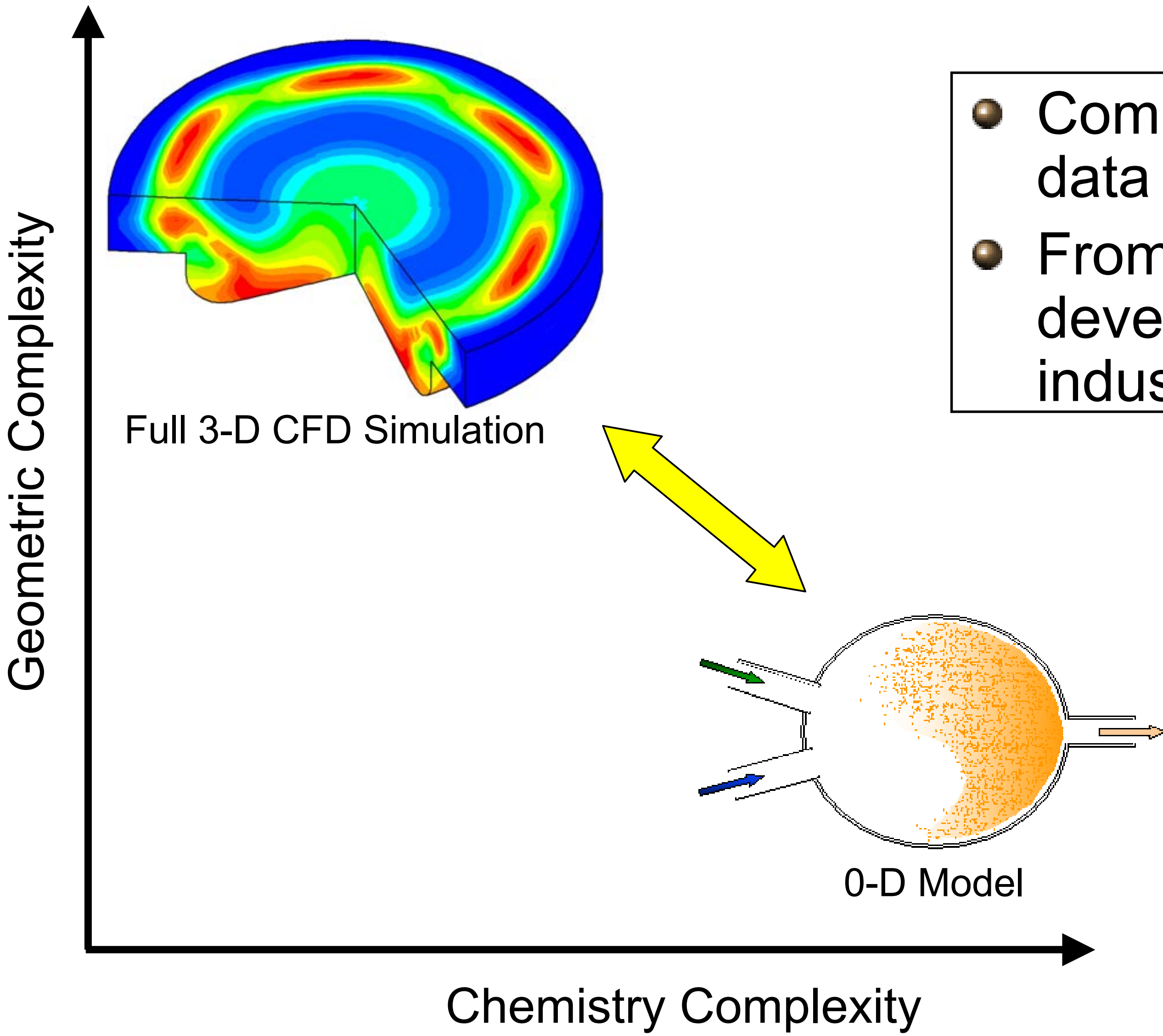
$$\text{rate} = \frac{k' C_A C_B}{\left(1 + K_A C_A + K_B C_B + K_C C_C + K_D C_D\right)^2}$$

  - Users enter *k'*, K_A, K_B, etc. directly
  - No user subroutine required
  - Allows direct use of plant data as well as comparison of detailed and global rate expressions

- New pressure-dependent reaction-rate formulation from Sandia National Laboratories
  - New mechanisms from J. A. Miller at Sandia Nat'l Labs
  - Interpolation of rates that are provided at several pressures

KINetics/API and links to 3rd-party Programs

Many problems require treatment of complex geometry and mixing limitations



- Common chemistry data descriptions
- From mechanism development to industrial design

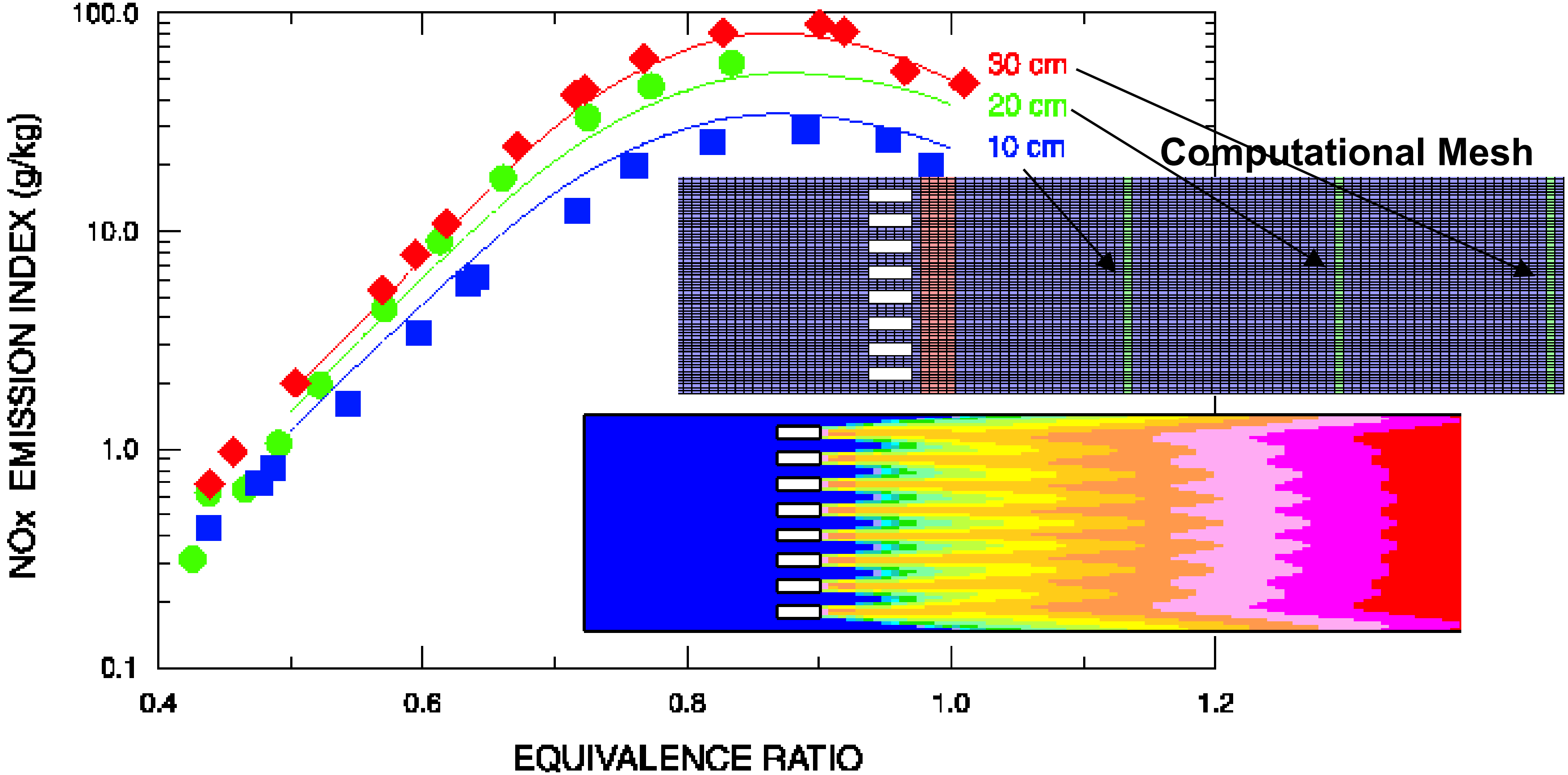
The KINetics module provides CHEMKIN technology as a plug-in to other programs

- Built-in transient and steady-state solution algorithms for CFD as well as 1-D flow-system modeling
  - Algorithms handle “stiff” chemistry within CFD
  - Accurate prediction of trace species
- Object-oriented modules with well documented API for linking to other programs
  - C++, C, F90, and F77 interfaces available
  - Dynamically linkable at runtime
- Complete compatibility with CHEMKIN
  - Thermochemistry and molecular transport
  - Gas-phase reactions
  - Gas-surface reactions on walls and in porous media

REACTION DESIGN

Link between STAR-CD and KINetics has been commercially available since 2001

STAR/KINetics Solver Predicts NO_x

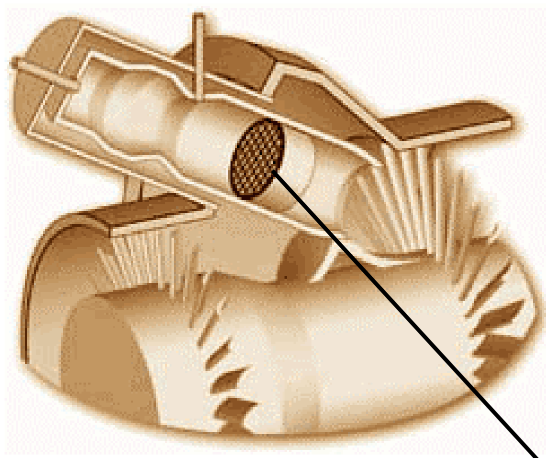


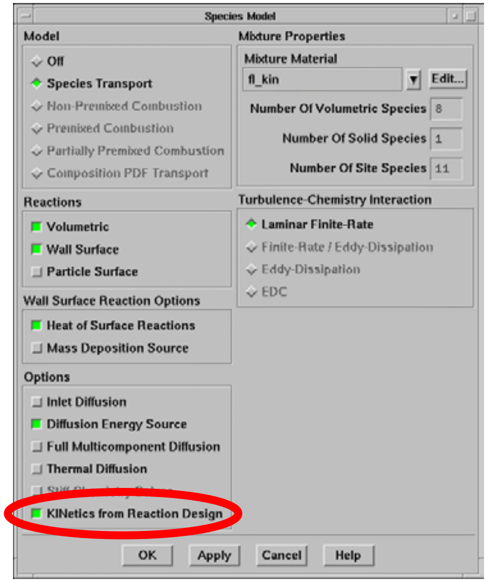
[1]Anderson, D.N., NASA-TM-X-71592, 1975

[2]Deur, J.M., et al., AIAA Paper 94-3895-CP, 1994

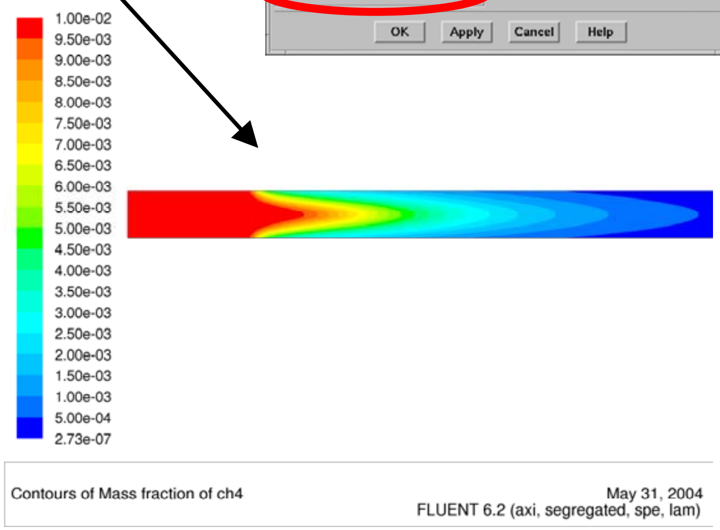
Reaction Design

Link between FLUENT and KINetics is scheduled for release in Q4’04





FLUENT/KINetics Simulation of Catalytic Oxidation of CH_4 on Pt in Monolith Channel for Two-stage Gas-Turbine Combustor



KINetics/API can be used to link to other 3rd-party and in-house tools

- Cell-by-cell simulation of chemistry allows robust treatment of stiff combustion and pollution-formation kinetics
- Allows linking to
  - Company in-house tools
  - Commercial CFD tools
  - Matlab or other mathematical simulation tools
  - 1-D engine-simulation tools
  - etc.

REACTION DESIGN

Model Fuels Consortium Initiatiave

Reaction Design is initiating an industry-driven consortium for engine simulation

- Designed to serve as a bridge to NIST Real Fuels and other database and mechanism development activities
- Focus on software tools and validation of mechanisms needed for practical engine simulation
- Based on premise that surrogate components can be identified to represent real-fuel mixtures

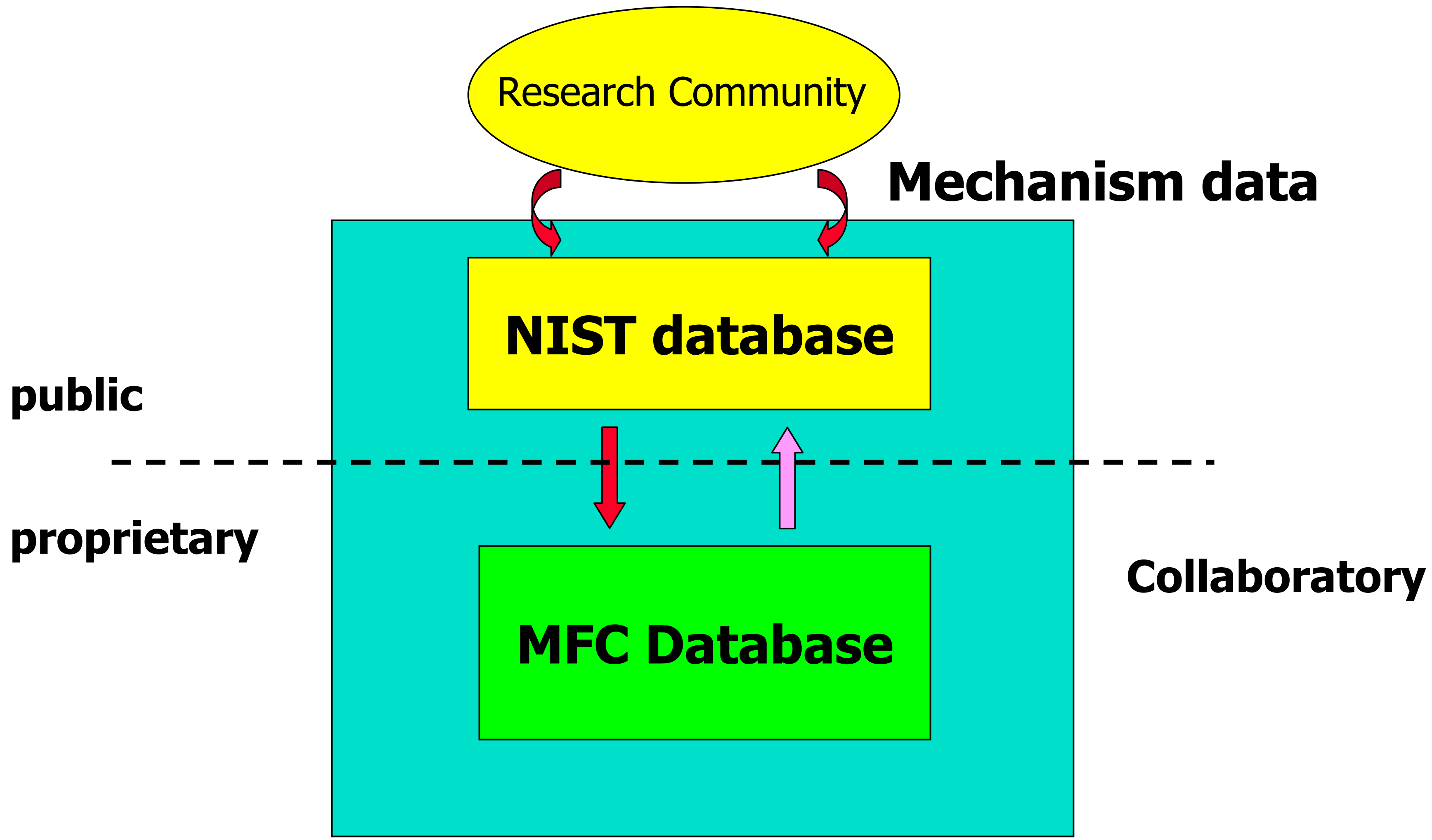
The consortium will focus on immediate payback from existing methodologies

- Commercial-grade software tools for analysis and simulation
- Mechanism assembly for detailed kinetics
  - Collaboration and partnerships with research groups
- Validation
  - Validation and optimization based on relevant engine and controlled experimental conditions
  - Experimental comparisons between surrogate and real fuel mixtures
- Mechanism reduction for practical engine design
  - < 50-100 species
  - Tools for automated mechanism reduction
- Coordination with NIST and other groups to bring in new science as it is developed
  - Funnel industry priorities to researchers

The consortium will drive tool and mechanism development for targeted applications

Mechanism Reduction and Analysis tools	Engine-simulation tools
Reduced models	Client proprietary mechanisms
Mechanism Database	

Collaborative Database Infrastructure



Expected start in Q4 '04

- Potential members include
  - Engine companies
  - Fuels and lubricants companies
  - Tier-one automotive suppliers
  - Government agencies
- Academic advisors
  - Prof. Anthony Dean, Colorado School of Mines
  - Prof. William Green, Massachusetts Inst. of Technology
  - Prof. Mitsuo Koshi, Tokyo University
  - Prof. Ulrich Maas, Universität Karlsuhe
- 3-Year project timeline

Future of this Workshop...

Questions we have for you

- Long-term goals for this workshop
  - Keep venue at Combustion Symposium?
  - Establish more regular “user-group” meeting?
    - » Where and when?
  - What format is best for the workshop?
  - What topics would you like to see covered?
- How can we help vitalize a Teaching-with-CHEMKIN forum?
  - On-line or face-to-face meetings?
  - How to seed exchange of sample problems?

Please fill out the survey to help us plan accordingly